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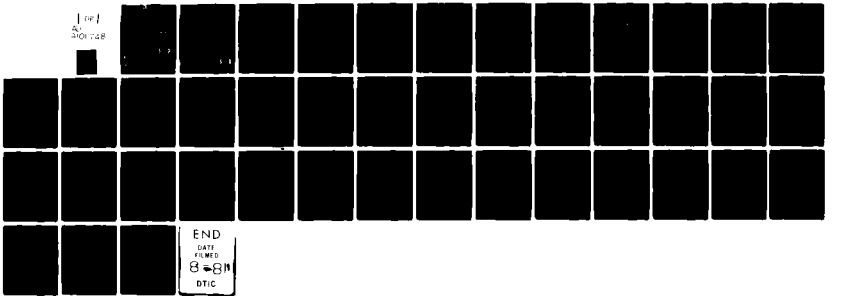

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A computer simulation investigation of a dynamic near-surface dislocation operation resulted in the formation of a hard layer of 10 to 500 μm in thickness. This hard layer disappears with time at room temperature when the stress has been removed, i.e. relaxation. The relaxation time for Cu is approximately 2 weeks; for Fe-Si and Mo the relaxation time is 2 and 10 years, respectively.

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SURFACE EFFECTS ON PLASTIC DEFORMATION

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by

R. J. Arsenault

and

I. R. Kramer

May 1981

Report No.

81-1

INTRODUCTION

The presence of a higher dislocation density in the near surface region of a material which has been plastically deformed and the stress removed can not be readily explained by any existing dislocation models. The primary goal of the present investigation is to develop a model which will account for a higher dislocation density in the near surface region.

The initial starting conditions of the proposed model are two valid assumptions: (1) Surface sources can be activated at a lower stress than sources in the interior of a sample. (2) Thermally activated dislocation motion from a source will create an inverse pile-up. Therefore, if all dislocations are generated from a surface source and their motion is controlled by thermal activation, then there will always be a higher dislocation density in the near surface region during loading. However, if the load, i.e. the stress, is removed the dislocation will have a tendency to escape from the material as a result of a combination of forces acting on the dislocations nearest the surface. These forces are: (1) Line tension due to the curvature of dislocation loop. (2) Attractive force by image dislocation arrays, which are mirror images to the real dislocations. (3) Repulsive forces by those dislocations of the same sign, lying ahead in the pile-up.

An assumption was made that some extra barriers would have to be introduced after deformation had begun which would stop the dislocations from exiting the material. The interaction of a secondary dislocation slip system with the primary one will create these extra barriers in f.c.c. metals.

The discussion of the results will be divided into several different parts.

DISCUSSION OF RESULTS

In order to attain the objective of the proposed research several different variations of the basic model, i.e. surface source operation of both primary and secondary slip planes, were investigated simultaneously. The following are the three models initially considered (there were numerous variation of each model):

1. In a real f.c.c. sample the dislocations in the primary and secondary slip systems do not interact at right angles. Therefore, it is necessary to consider a three dimensional model with two intersecting slip planes. The static interaction between various configurations of two systems of nonparallel, noncoplanar straight edge dislocations of slip system $[10\bar{1}]$ $(\bar{1}2\bar{1})$ and $[0\bar{1}\bar{1}]$ $(\bar{2}1\bar{1})$ are being considered. The probability of doing a computer simulation of dislocation motion of this three dimensional model is remote. However, the interaction forces between dislocations can be obtained, which can be used in a two or more dimensional dynamic models.

2. A two dimensional model with two slip systems: Two systems of parallel-straight-edge dislocations lying on two slip planes intersecting at 70° which can operate simultaneously from each surface source. In this model consideration of dislocation motion is possible. In addition, line tension terms are included which take into account the circular nature of dislocation loops. Also, the image forces are considered.

3. A one-dimensional model with one slip system: A group of straight-edge dislocations parallel to each other are created from a surface

source and move on a slip plane by an applied shear stress. This model would require the least amount of computer time.

Model 1

In FCC metals, edge dislocations on the secondary and primary slip planes are never parallel to each other. In order to represent the real orientation, a three dimensional model is needed (Fig. 1). The interaction force between the primary and the secondary dislocations is thus the general case of a non-parallel, non-coplanar dislocation pair. The correspondence of this three-dimensional model and the previous two-dimensional model can be understood by looking at the viewing plane perpendicular to the intersection line $\bar{MN}$, (Fig. 2) with the dislocation penetration spots P and S considered as the equivalent two-dimensional dislocation locations. Therefore, when the two dislocations are equidistant to the junction point 0 and are on the same side from 0, they are actually intersecting each other along MN somewhere. As the dislocations intersect each other, an attractive junction should have formed which would require approximately 10^2 eV to break them apart in either direction.

An interesting fact is that the total interaction force between a general dislocation pair is independent of the nearest distance between them. As the dislocations approach each other, the interaction region simply becomes more localized with higher force per unit dislocation length near the points of smallest distance. An attempt is made to simplify the model by considering only the length of dislocation with an interaction force per b greater than some threshold value. Since the total force is a constant, as the dislocations approach each other, the effective length become smaller and the effective interaction force per b will thus increase. It turns out

that the effective length is a linear function of the nearest distance. The attractive force toward the junction on both planes seems to agree with the attractive junction formation arguments. The information from this model was put into Model 2.

Model 2

The two dimensional model is based on the dynamic (thermally activated) motion of parallel edge dislocations moving on two intersecting slip planes at an angle α, as in Fig. 3. For FCC metals,{111} slip planes intersect at $\alpha=70°$. For each dislocation present, the interaction with all other dislocations and their images on both planes have to be considered (Fig. 4). The applied stress component on the secondary slip plane is determined from the Schmid factor which corresponds to a maximum probability of secondary slip. A number of static interaction for various dislocation configurations has been studied. The dislocations on the primary and the secondary systems seem to be moving in a cooperative mode. As the leading dislocations approach the junction on their respective plane, they encounter increasingly large repulsive forces. Therefore, it seems that if both systems are to be operated simultaneously, they will block each other at the junction.

If the inverse pile-up already existed on the primary plane when the secondary system is activated, the result indicate that there are open-gate and close-gate configurations for the primary dislocations. In other words, the secondary dislocations can easily move through the junction if the primary dislocations are preferentially distributed; whereas in closed gate, it will be extremely difficult to pass it. In the closed gate case only the primary slip system operates, but in both cases a higher dislocation density exists in the near surface region.

If the stress is removed from the case where both slip systems operate (i.e. open gate) then a finite number of dislocations leave the sample, but the rate is very slow.

Model 3

This model involves the motion of dislocations from a source on a single slip plane. The motion is controlled by the thermally activated jumping of discrete short range barriers (SRB) or a friction model. The details of these two cases are described in the two attached papers. The conclusions obtained from the investigations based on the one dimensional model are as follows:

1. A dynamic inverted dislocation pile-up occurs for the three metals investigated, Cu, Fe-Si and Mo.

2. There is general agreement between the computer simulation results which show a higher dislocation density in the near surface region and dislocation etch pit studies which also show a higher dislocation density in the near surface region.

3. The dynamics of the dislocation motion were considered by two different models, thermally activated jumping of random short range barriers and a friction model. There is a larger dislocation density in the near surface region for the barrier model.

4. The maximum dislocation density increases when comparing Cu to Fe-Si and Fe-Si to Mo, but the width of the hard layer decreases when going from Cu to Fe-Si to Mo.

5. The increase in dislocation density in the near surface region decreases as a function of time when the stress has been removed, i.e. relaxation. The relaxation time for Cu is approximately 2 weeks, and for Fe-Si and Mo the relaxation time is about 2 to 10 years.

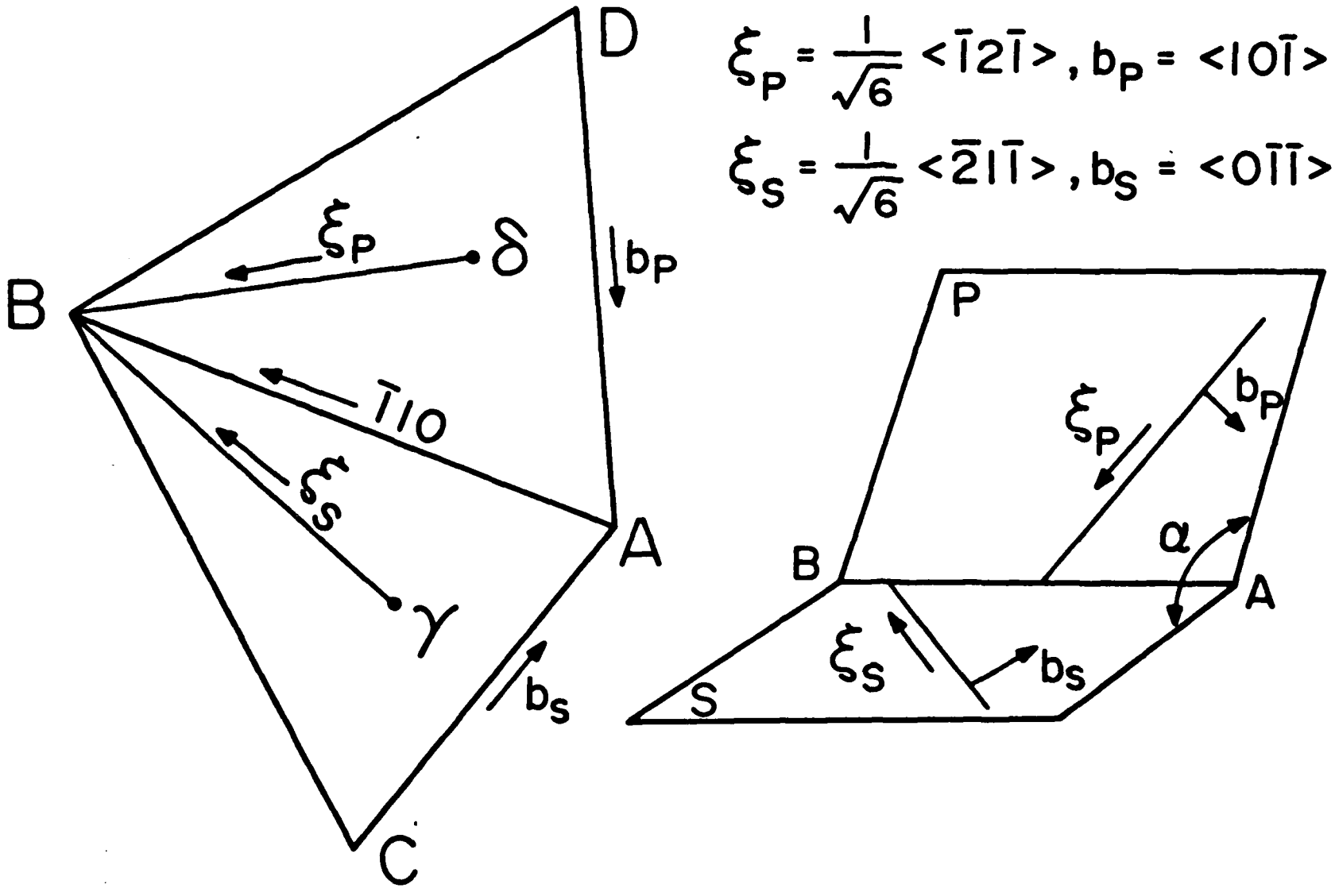

Fig. 1. A three-dimensional model of two slip systems.

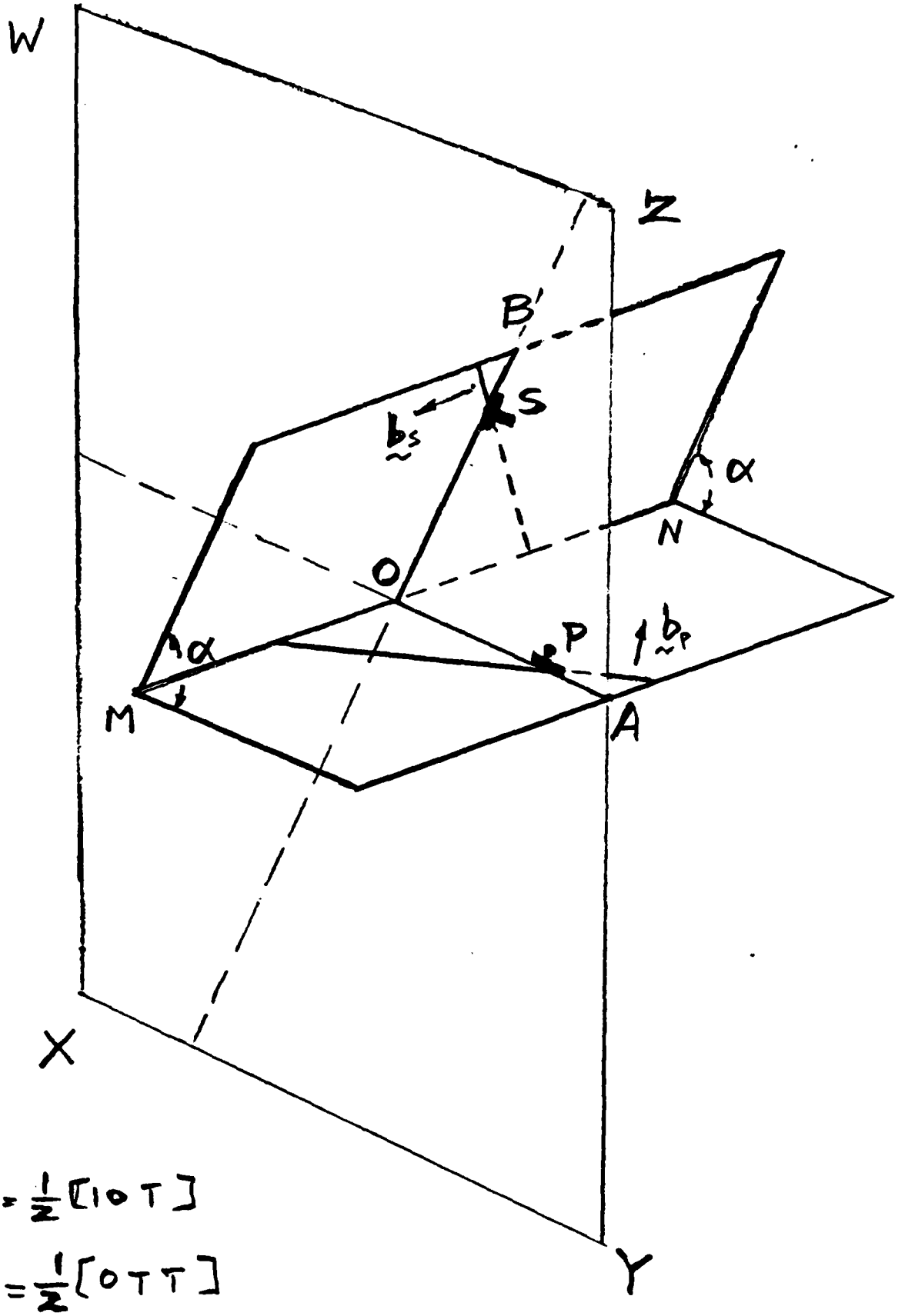

Fig. 2. The correspondence between 2- and 3-dimensional models.

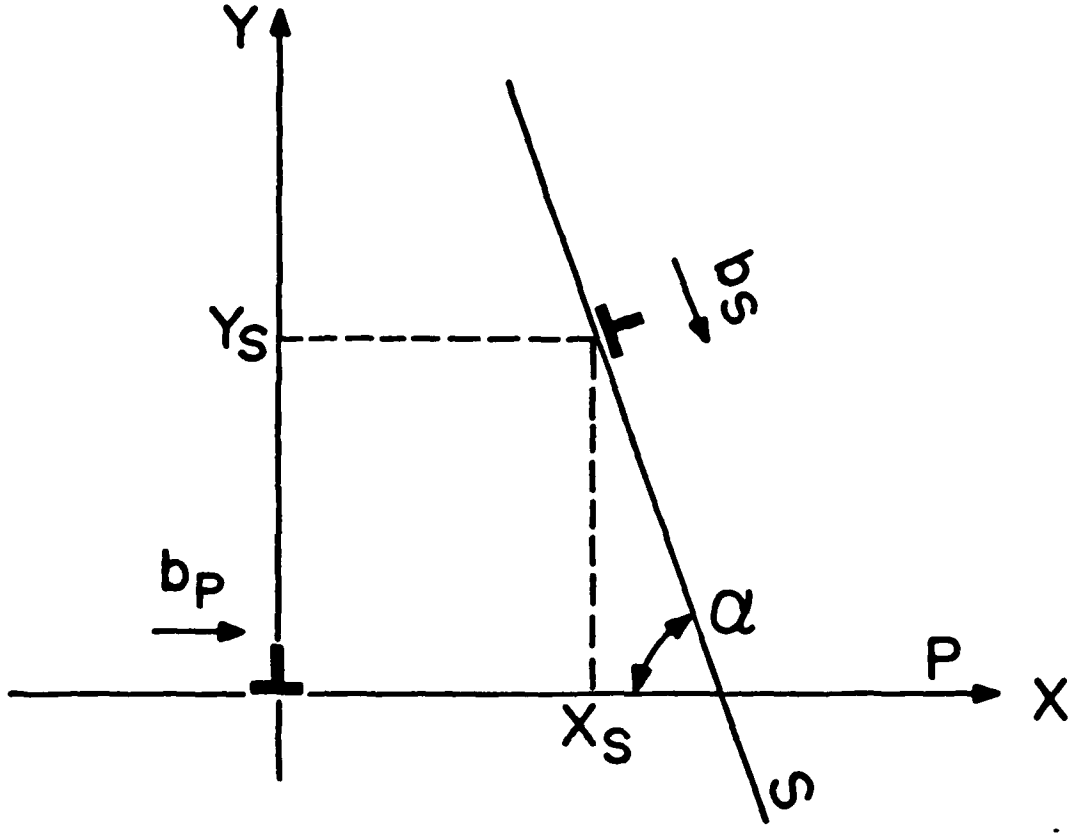

Fig. 3. Interaction between dislocations on the primary and secondary slip planes.

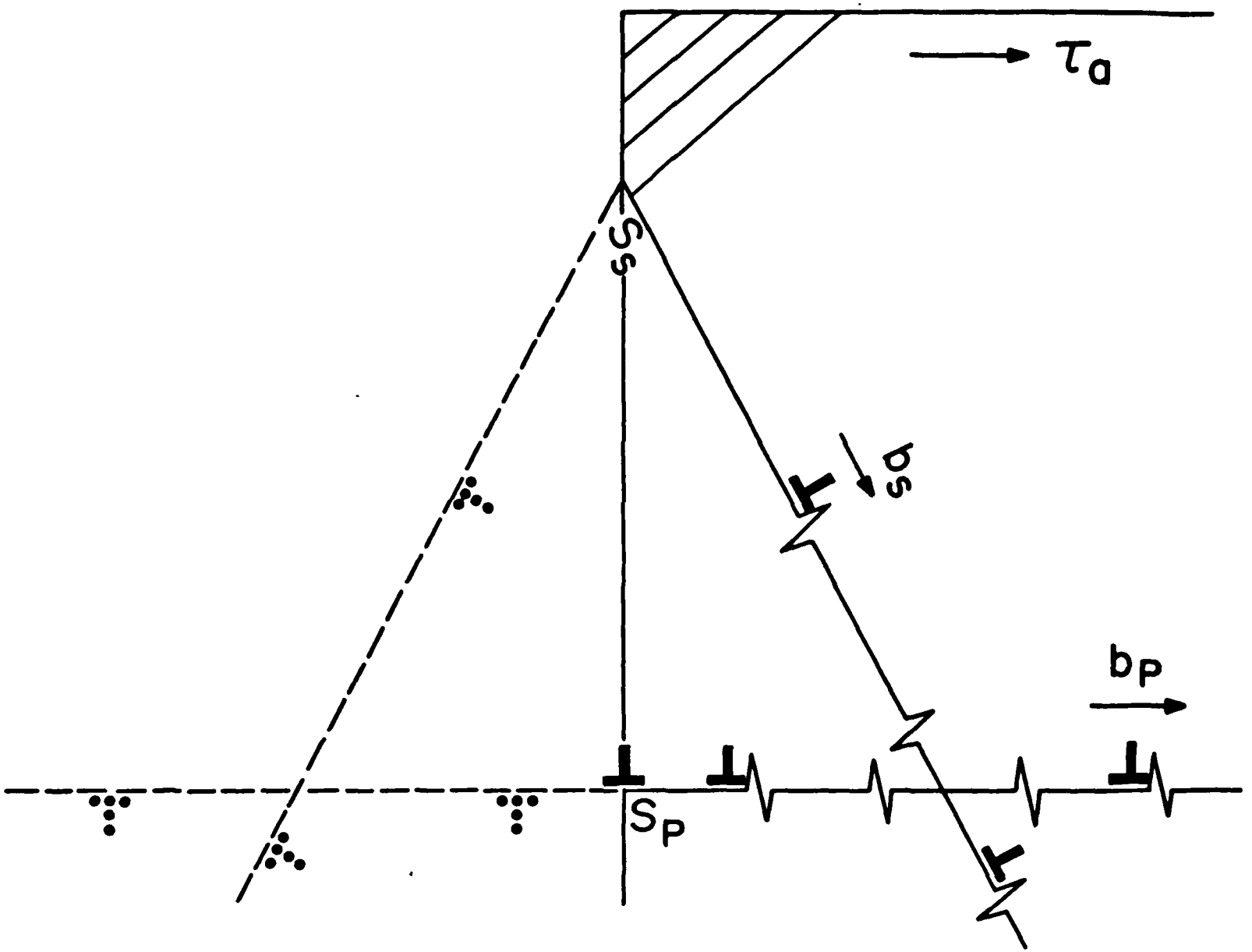

Fig. 4. A two-dimensional model with two slip systems and their image dislocations.

THE VELOCITY OF A GROUP OF DISLOCATIONS

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THE VELOCITY OF A GROUP OF DISLOCATIONS

R. J. Arsenault
R. Hsu

Introduction

In recent years, there have been several published reports on the motion of a group of dislocations generated from a continuously operating source (1-4). The general conclusion was that the velocity of the first dislocation generated was no more than a factor of three greater than that of a single dislocation traversing the same slip plane, with the same applied stress acting on the dislocation. Arsenault and Kuo (1)mentioned briefly that the average velocity of the dislocations generated from the source was the same as the velocity of a single dislocation. A corollary of this would be that, if the applied stress were zero, then the velocity of a single dislocation would be zero. One could then ask the question: Is the average velocity of a group of dislocations zero when the applied stress is zero?

This study was undertaken to determine if indeed the average group velocity is the same as that of a single dislocation at several different temperatures and stress levels in both the barrier and the friction models. Three different metals, Cu, Fe-Si and Mo were studied.

Procedure

All procedures were performed according to the methods previously described by Arsenault and Cadman (4) and Arsenault and Kuo (1), with modifications indicated in detail where necessary.

The first of two models used to study the motion of the dislocations was the thermally activated jumping of barriers. The motion

of dislocations from the source was treated as a one-dimensional problem in both models. In this case, the barriers were placed randomly in a row, and the strength of the barrier was a constant. The activation energy to jump the i^{th} barrier was defined by the following equation:

$$\Delta G_i = \Delta G_o \left[1 - \left(\frac{\tau_i^*}{\tau_o^*}\right)^{n_1}\right]^{n_2} \qquad (1)$$

where ΔG_o is the activation energy required to jump the barrier with τ_i^* equal to zero; n_1 and n_2 are constants that are determined from the experimental data; and τ_o^* is the stress required to jump the barrier at 0 K. The effective stress τ_i^* was given by

$$\tau_i^* = \tau_a + A \sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{1}{x_j - x_i}$$

where τ_a is the applied stress; N is the total number of dislocations; $A = \frac{\mu b}{2\pi(1-\nu)}$, μ is the shear modulus; b is the Burgers vector; and ν is Poisson ratio.

The terms in eqn 1, such as ΔG_o, n_1, n_2, τ_o^*, as well as the spacing between barriers and τ_a, were obtained from the experimental data of Kitajima (5) and Mitchell and Thornton (6) for Cu single crystals. In the case of Fe-Si, the parameters of eqn. 1 were obtained from the data of Stein and Low (7) as analyzed by Arsenault and Cadman (4). It was not feasible to perform simulation tests for Mo with the barrier model because of the computer time involved.

The source operation was conducted in the following manner. When τ^* was greater than τ_s at the position of the source, then a

dislocation appeared at the source. The dislocation moved (at drag velocity) until the τ^* on the dislocation was zero or until it met the first barrier. A check was then made to determine if $\tau^* > \tau_s$ at the source; if so, then another dislocation appeared at the source. When $\tau_i^* < \tau_s$, then the dislocations previously generated moved so that τ^* at the source position increased to τ_s. The binomial distribution method was used to determine the jump time. After a dislocation jumped, the τ^* on all dislocations were redetermined and positions of the dislocations between barriers were adjusted so that τ^* was zero on these dislocations. This process was repeated until a finite number of dislocations appeared on the slip plane. The methods for determining the dislocation positions and the velocities of the individual dislocations have been described elsewhere (8,9).

A second model, the friction model, was developed to reduce the amount of computer time. This model uses the following well-known eqn. relating dislocation velocity to stress:

$$v_{i-N} = Z(\tau_i^*)^{m^*} \qquad (2)$$

where v_{i-N} is the velocity of the i^{th} dislocation in the group of N dislocations and τ_i^* is the effective stress on the i^{th} dislocation and is determined in the same manner as it is in the barrier case and Z and m* are empirical constants. In the case of Mo, with a barrier spacing of 1 b, it was not feasible to do simulation tests with the barrier model. The values for Z and m* were obtained by replotting the experimental data of Hasson et al. (10).

Two different methods were used to conduct the simulation tests. 1) A given value of applied stress was imposed for a given length of time, and the velocity of each dislocation generated was determined. 2) A plastic strain rate $\dot{\varepsilon}_p$ was chosen, and then τ_a was adjusted to maintain a constant average $\dot{\varepsilon}_p$. The simulation tests were conducted at several different temperatures and stress (or $\dot{\varepsilon}_p$) levels.

The procedures used for the $\tau_a=0$ situation were basically the same as for a finite τ_a, with a few exceptions. In the case of $\tau_a=0$, there was a given dislocation arrangement (in general an inverted pile-up, but other arrangements were investigated); then the velocities of the individual dislocations were determined in both the barrier and the friction models.

Results and Discussion

The results obtained from both the constant stress and constant strain rate modes for the three different metals in the barrier and friction models were in agreement.

The velocity of the first dislocation (v_{1-N}) generated by the source was greater than that of a single dislocation (v_1). The ratio of V_{1-N} to v_1 was a function of temperature and applied stress, but the value was always less than 3. The velocity of the last dislocation generated (V_{N-N}) was always less than v_1. However, the average velocity ($\bar{v}_N$) of the group of dislocations which were generated by the source was equal to the velocity of a single dislocation. If $\bar{v}_N$ were not equal to v_1 then it would be necessary to define or determine the velocity of each of the mobile dislocations.

The fact that $\bar{v}_N$ was equal to v_1 is important, for it has been assumed that the plastic strain rate can be defined as follows:

$$\dot{\varepsilon}_p = \bar{v}_N \rho b \qquad (3)$$

where ρ is the density of mobile dislocations.

When τ_a=o, the velocity of a single dislocation was zero. The algebraic average of the velocity of the group of dislocations was also zero when τ_a=o. This means that some dislocations within the group were moving forward and some were moving backwards. The result, i.e., $\bar{v}_n$ = o when τ_a = o, was independent of metal or model.

Conclusions

These data, obtained from a series of computer simulation tests, indicate that the average velocity of a group of dislocations generated from a source is equal to the velocity of a single dislocation traversing the same slip plane and, when the applied stress is zero on a group of dislocations, the average velocity of this group is zero.

Acknowledgement

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Deformation - Dislocation

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A HARD SURFACE LAYER* R. J. Arsenault, R. Hsu, University of Maryland, College Park, Md. 20742

There are numerous experimental observations which indicate that the dislocation density is higher in the near surface region of a sample which has been plastically deformed. An investigation was undertaken to develop a dislocation mechanism which could account for a higher dislocation density in the near surface region of a sample which had been plastically deformed. A computer simulation study of the operation of a near surface dislocation source, based on thermally activated dislocation motions, indicated that a higher dislocation density is possible. The computer simulation results indicate that the higher density extends to a depth of 100 μm in Cu, and this compares with etch pit dislocation density measurements which indicate a depth of ~ 60 μm. Computer simulation studies of Fe-Si and Mo indicate a higher dislocation density in the near surface region. The dislocation density is larger than that obtained for Cu.

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OPERATION OF NEAR SURFACE DISLOCATION SOURCES

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OPERATION OF NEAR SURFACE DISLOCATION SOURCES

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ABSTRACT

Numerous experimental observations have suggested that there is a higher dislocation density, i.e. a hard layer, in the near surface region of a plastically deformed sample. In this study, we considered a possible dislocation model which can account for this hard layer. A computer simulation investigation of a dynamic near-surface dislocation operation resulted in the formation of a hard layer of 10 to 500 μm in thickness. This hard layer disappears with time at room temperature when the stress has been removed, i.e. relaxation. The relaxation time for Cu is approximately 2 weeks; for Fe-Si and Mo the relaxation time is 2 and 10 years, respectively.

INTRODUCTION

The arrangment and density of dislocations in the near surface region affect important properties of materials, e.g. fatigue, stress corrosion cracking, friction and wear, etc. Kramer and co-workers (1,2) reported an increase in the density of dislocations in the near surface region (i.e. to

a depth of ~ 100μ) in samples that were deformed in tension or in tension-compression fatigue. This increase in dislocation density in the near surface as compared with the interior of the sample is defined as the "hard layer" phenomenon. Support for the hard layer pheonomenon can be found in investigations in which transmission electron microscopy (3-5), etch pits (6-10) and a birefringent technique (11-12) were used.

In a simple tensile test, the dislocation density decreases to a constant value as the depth beneath the surface increases. However, in the case of samples subjected to tension-compression fatigue, the dislocation density decreases, attains a minimum, then increases to a constant value as the depth beneath the surface increases. This increase in dislocation density was determined by an X-ray technique (13). In addition, this double crystal diffraction X-ray technique was used to determine the density of dislocations of one sign in excess of the density of dislocations of the opposite sign. For example, when the density of positive dislocations is 5×10^8 cm^{-2} and the density of negative dislocations is 3×10^8 cm^{-2}, the density determined by this technique is 2×10^8 cm^{-2}.

Kitajima and co-workers (6) have conducted extensive dislocation etch pit experiments. They have shown that a higher dislocation density exists in the near surface region, and they have produced plots of dislocation density vs distance into samples , which have been deformed by various amounts. They also have determined the activation volume and

energy for plastic deformation from the same samples. From the activation volume data it is possible to calculate the spacing between the short range barrier i.e. the barriers jumped by thermal activation. If the density of forest dislocations is related to the measured density, and if the forest dislocations are the short range barriers, then the density of the short range barriers would be comparable to the measured dislocation density. Therefore, it is possible to check values reported for the activation volume.

It has been argued that this increase in dislocation density is due to a strong adherent oxide layer on the metal (14). However, it has been shown that an increase in the dislocation density in the near surface region occurs in Au single crystals also (15). One possible explanation for the existence of a hard layer in metals that have a strong adherent oxide layer can be found in a dislocation pile-up model at the oxide-metal interface. The stress field of this dislocation pile-up would activate secondary sources near the surface, which would then result in an increase in dislocation density, i.e a hard layer.

Fourie (16) has obtained data which strongly suggests that the surface region of a deformed sample has a lower dislocation density than that in the interior of the sample, i.e. a "soft layer". The data supporting the concept of a soft layer has been reviewed in detail by Nabarro (14).

An elastoplastic model can be used to explain a soft

layer (17). If a cylinder of uniform cross-section were loaded in tension, then the central core would be subjected to a higher stress. If the dislocation sources were uniformly distributed in the sample and the same stress was required to operate all of them, then the central core region would yield first and then gradually harden to a greater extent than the surface region, i.e. a softer outer layer. Also, the image forces on a dislocation would be important in reducing the dislocation density near the surface, which again would result in a softer outer layer.

As another argument against the presence of a hard layer, Nabarro (14) cites the experimental observation by Kramer (18) that the hard layer can relax in some materials, e.g. copper, within a relatively short time (2 weeks at room temperature), which suggests that the activation energy for the process is low (12.6 KJ/Mole). However, in the case of Fe-Si, there is no detectable relaxation of the hard layer at room temperature. The question of this relaxation phenomenon remains unanswered.

To date, no complete mechanism for the presence of a hard outer layer in metals without a strong adherent oxide has been proposed. It has been suggested that the stress required to operate Frank-Read sources is less in the near surface region, e.g. the Fisher mechanism (19). There is also the possibility that the mesh length of the Frank net is longer in the near surface region than in the interior, which would mean that the stress needed to activate these sources

would be less than that required to activate the sources in the interior of the sample. Nevertheless, there is still the problem of how this high density continues to exist in the near surface region when the stress is removed, since the image and line tension forces would be acting to remove dislocations from the near surface region.

In the present study, we consider whether a near surface source operation would result in a higher dislocation density in the near surface region.

PROCEDURE

The proposed model for a higher dislocation density in the near surface region is based on two valid assumptions: i. The stress required to operate a source in the near surface region is less than that required to operate a source in the interior of a sample; and ii. the motion of the dislocations is controlled either by a thermally activated "jumping" of discrete barriers, or by a "frictional" force.

The motion of edge dislocations from the source is treated as a one-dimensional problem. The procedure used is similar to that described by Arsenault and Cadman (20) and Arsenault and Kuo (21), with modifications detailed as necessary. The model used for dislocation motion controlled by thermally activated jumping will be described first and then the "friction" model.

In the one-dimensional case, the barriers are placed randomly in a row and the strength of the barrier is a constant. The activation energy necessary to jump the i^{th}

barrier is defined by the following eqn.

$$\Delta G_i = \Delta G_o \left[1 - \left(\frac{\tau_i^*}{\tau_o^*}\right)^{n_1}\right]^{n_2} \tag{1}$$

where ΔG_o is the activation energy required to jump the barrier than τ^* is zero n_1 and n_2 are constants which are determined from the experimental data, and τ_o^* is the stress required to jump the barrier at O K. The effective stress τ^* is defined as follows:

$$\tau_i^* = \tau_a + A \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{1}{x_i - x_j} - \tau_\Gamma - \tau_I \tag{2}$$

where τ_a is the applied stress, $A = \frac{\mu b}{2\pi(1-\nu)}$, N is the total number of dislocations, μ is the shear modulus, b is the Burgers vector, ν is Poisson's ratio, τ_Γ is the line tension term and τ_I is the image term which shall be described in detail later.

If the dislocation source is within the interior of the sample, there is no image term. Also, previously it was assumed that the source was an infinitely long straight dislocation, so there was no line tension term. The effect of changes in the source operating stress was reinvestigated and again, within reasonable limits, changes in this stress had very little effect on the velocity ratios of the dislocations involved and the arrangement of these dislocations.

A determination of the image stress of an edge dislocation

is not a simple matter. However, Head (22) has developed an expression for the stress field of edge dislocation near a free surface so that it is possible to use the following simplified formula for dislocations on the same slip plane:

$$A \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{1}{x_i - x_j} - \tau_I \tag{3}$$

$$= A \left\{ -\frac{1}{2x_i} + \sum_{\substack{j=1 \\ j\neq i}}^{N} \left[\frac{1}{x_i - x_j} - \frac{1}{x_j + x_i} + \frac{2x_i(x_i - x_j)}{(x_j + x_i)^3} \right] \right\}$$

where the terms on the right side of the above eqn are those developed by Head (22), and x_i and x_j are the distances from the free surface of the i^{th} and j^{th} dislocations.

The line tension term was determined by assuming that the chosen source operating stress (τ_s) defines a given Frank-Read source length, and also that the dislocation bows out as the arc of a circle. The τ_Γ can be defined by the following equation:

$$\tau_\Gamma = \frac{\Gamma}{Rb} \tag{4}$$

where τ is the line tension which is equal to $\frac{\mu b^2}{2}$, and R is the radius of the dislocation arc.

For copper, the terms in eqn 1, e.g. ΔG_o, activation volume, the spacing between barriers and τ_a were obtained from the experimental data of Kitajima et al. (7), and the value

of τ_o^* used is that given by Mitchell and Thornton (23). In the case of Fe-Si, the data of Stein and Low (24) as analysed by Arsenualt and Cadman (20) were used to obtain the parameters n_1 and n_2 of eqn. 1. A summary of the parameters used are given in Table I.

The method of source operation is as follows: If τ^* is greater than τ_s at the position of the source, then a dislocation comes into existence at the source. The dislocation moves until the τ^* on the dislocation is zero or until it meets the first barrier. The first dislocation generated meets the first barrier, but there is a finite possibility that the second dislocation is generated before the first dislocation jumps the barrier, which means that there is perhaps more than one dislocation positioned between barriers.

The τ_i^*, ΔG_i and the time required to jump the i^{th} barrier are determined for each dislocation against a barrier. The jump times were determined by the binomial distribution method and the dislocation which is to jump was selected by a Monte Carlo technique. This process was repeated until a finite number of dislocations had come into existence on the slip plane. The method for determining the dislocation positions and the velocities of the individual dislocations has been described elsewhere (25).

The dislocation density was determined by counting the number of dislocation within a given length (ΔL) along a slip plane. The various ΔL values used for the different materials are listed in Table I. The average slip plane

separation was determined from etch pit studies.

The total number of dislocations (N) generated for a given set of conditions was determined by increasing the number generated until at some distance beneath the surface the density did not change with further increases in number of dislocations generated. The number generated is a function of the material and the applied stress (or $\dot{\varepsilon}_p$) levels, and they are listed in Table II.

The simulation tests were conducted in two different modes: 1.) A given value of applied stress was imposed for a given length of time; then applied stress was removed, and the dislocation arrangement was allowed to relax. ii) A plastic strain rate $\dot{\varepsilon}_p$ was chosen; then τ_a was adjusted to maintain a constant $\dot{\varepsilon}_p$; and again, τ_a was removed and the dislocation arrangement was allowed to relax.

The friction model was developed to reduce the amount of computer time. In the case of Mo, with a barrier spacing of 1 b, it was not feasible to do simulation tests using the barrier model. The friction model employs the following well-known eqn. relating dislocation velocity to stress:

$$v_i = B(\tau_i^*)^m \tag{5}$$

where v_i is the velocity of the i^{th} dislocation, τ_i^* is the effective stress on the i^{th} dislocation and is determined in

the same mammer as for the barrier case, and B and m are constants. The dislocation source is operated in the same manner as that for the barrier model.

RESULTS AND DISCUSSION

The activation of the near surface dislocation sources results in the formation of a dynamic inverted dislocation pile-up. The discussion of the specifics of the result is divided into four categories.

1. A Comparison of the Simulation and Kitajima Data.

A detailed comparison between experimental data and computer simulation results is possible for the case of the etch pit data of Cu generated by Kitajima (7).

Fig. 1 shows a plot of the Kitajima data of dislocation density vs distance into the center of the sample, and Fig. 2 shows the data obtained for a constant applied stress simulation test. The simulation results were obtained from the barrier model as soon as the applied stress was removed. Although the Kitajima data and the simulation data generally agree there are some differences, for example, the thickness of the "hard layer" is greater in the simulation data than in the experimental data.

2. A Comparison of the Barrier and Friction Models.

A comparison of the dislocation density vs distance relationship for the barrier and friction models can be made for Cu and Fe-Si. The data in Fig. 3 are representative of the differences between the two models. For a given ex-

ternal stress, the density of dislocation in the "hard layer" is greater in the barrier model than in the friction model. However, the differences (Fig. 4) between these two models, especially in the case of Fe-Si could be due to the local fluctuations in dislocation density as a result of random barrier spacing. There is also a larger number of dislocations behind the barriers near the source than at barriers farther from the source. The net result is that there is a larger dislocation density in the near surface region from the barrier model.

3. A Comparison of Cu, Fe-Si and Mo.

In all cases a "hard layer" forms, but the extent, i.e. the density of the dislocations and the thickness of the near surface region, depends upon the metal under consideration. The maximum density increases when comparing Cu to Fe-Si and Fe-Si to Mo as shown in Table II. However, the width of the hard layer decreases when going from Cu to Mo and to Fe-Si.

The apparent hard layer thickness can be determined from the dislocation density vs distance curves. The hard layer can be determined by arbitrarily choosing a position where change in density with distance became small, i.e. approaching an asymptotic value. In this study the hard layer thickness was defined as the position where the dislocation density was $1/5\ (\rho_l^{max} - \rho_l^{min}) + \rho_l^{min}$, where ρ_l^{max} is the maximum dislocation density at the surface and ρ_l^{min} is the minimum dislocation density in the interior of the sample. A summary of hard layer thicknesses is given

in Table II.

The number of dislocations generated in order to determine the asymptotic value depended upon the stress and metal under consideration, but in general the number increased from Cu to Fe-Si to Mo. In the case of Mo more than 80 dislocations were required to approach the asymptotic value.

For Mo, the dislocation density profiles were determined at several temperatures. At the same constant strain rate of 1.67×10^{-5}/sec, the dislocation density distribution vs the depth from surface was about the same within the temperature range of 192K to 298K. This finding does not agree with Kramer's finding (18) that the surface stress decreased linearly as the temperature increased.

4. Dislocation Relaxation.

When the previously loaded samples are unloaded for given periods of time, the hard surface layer gradually disappears, i.e. the dislocation density near the surface decreases with time when $\tau_a = 0$. This disappearance of the hard surface layer at $\tau_a = 0$ is defined as "relaxation". The reasons for this relaxation phenomenon are as follows: Although the dislocations furthest away from the surface are nearly straight, those dislocations near the surface source should have a smaller radius of curvature, i.e., as an arc of a circular loop. The isotropic approximation of the dislocation energy per unit length is termed "line tension," which has a backward component tending to pull the dislocations out of the crystal. There are also image

forces to attract dislocations to the surface. In addition, all of the dislocations further away from the source push the dislocations near the surface backward.

This room temperature relaxation phenomenon may explain why the hard surface layer was not found in some experimental studies, particularly in those metals with a very short relaxation time. In the case of Cu, the simulation results indicated a relaxation time of two weeks at room temperature, which agrees well with Kramer's (18) experimental results. As for Fe-Si and Mo, the relaxation time is 2 years and 10 years, respectively.

CONCLUSIONS

From this computer simulation investigation of dynamic near surface dislocation source operation, it was possible to arrive at the following conclusions:

1. A dynamic inverted dislocation pile-up occurs for the three metals investigated, Cu, Fe-Si and Mo.

2. There is general agreement between the computer simulation results and the dislocation etch pit studies, which both show a higher dislocation density in the near surface region.

3. When we considered the dynamics of the dislocation motion by using two different models, thermally activated jumping of random short-range barriers and a friction model, we found that there is a larger dislocation density in the near surface region for the barrier model.

4. The maximum dislocation density increases when comparing Cu to Fe-Si and Fe-Si to Mo, but the width of the hard layer decreases when going from Cu to Mo to Fe-Si.

5. The increase in dislocation density in the near surface region decreases as a function of time when the stress has been removed, i.e. relaxation. The relaxation time for Cu is approximately 2 weeks, and for Fe-Si and Mo the relaxation time is 2 to 10 years.

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TABLE I

ROOM TEMPERATURE PARAMETERS USED FOR VARIOUS MATERIALS

MODEL	PARAMETERS	MATERIAL		
		Fe-Si	Mo	Cu
BOTH BARRIER AND FRICTION	Shear Modulus μ [MPa]	7.73×10^4	1.22×10^5	4.0×10^4
	Yield Stress at 0°K, τ_o^* [MPa]	3.9×10^2	6.0×10^2	4.0
	Dislocation Density Measurement Length, ΔL [b]	$2 \sim 5 \times 10^4$	5×10^4	5×10^5
	Source Operating Stress, τ_s [MPa]	4.0×10^{-2}	1.0×10^{-1}	4.0×10^{-2}
FRICTION	ln B	-45.415	-25.643	2.851
	m	9.968	4.847	8.665
BARRIER	n_1	0.5	0.5	0.6
	n_2	2.0	1.2	3.2
	ΔG_o [KJ/mole]	109	116	84.3

TABLE II

COMPARISON OF DISLOCATION DISTRIBUTION FOR

DIFFERENT MATERIALS IN EACH MODEL

MODEL	SIMULATION RESULTS	MATERIAL		
		$Fe\text{-}S_i$	Mo	Cu
BARRIER	Hard Layer Thickness, [μm]	10	-	125
	Maximum Dislocation Density [cm^{-2}]	3.4×10^{7}	-	5.6×10^{5}
	Number of Dislocations to Reach Core Region	40-50	-	30
	Maximum Dislocation Penetration, [b]	2.5×10^{5}	-	1.9×10^{7}
FRICTION	Hard Layer Thickness [μm]	40	125	500
	Maximum Dislocation Density [cm^{-2}]	2.3×10^{6}	1.1×10^{7}	1.6×10^{5}
	Number of Dislocations to Reach Core Region	40-60	60-80	30-40
	Maximum Dislocation Penetration [b]	2.8×10^{6}	1.2×10^{6}	1.16×10^{7}

Figure Captions

Fig. 1. Kitajima's experimental data of dislocation densities vs. distance beneath the surface, for plastically deformed Cu single crystals at the beginning of macro yield point and during stage I, respectively.

Fig. 2. The effect of different levels of applied stress for the barrier model of Cu, at 298K, with 30 dislocations generated in each case.

Fig. 3. The comparison between the barrier and the friction models for Cu at constant τ_a = 1 MPa, 298K, with 30 dislocations generated in each case.

Fig. 4. The comparison between the barrier and the friction models for Fe-Si at constant $\tau_a = 10^2$ MPa, 298K, with 40 dislocations generated in each case.

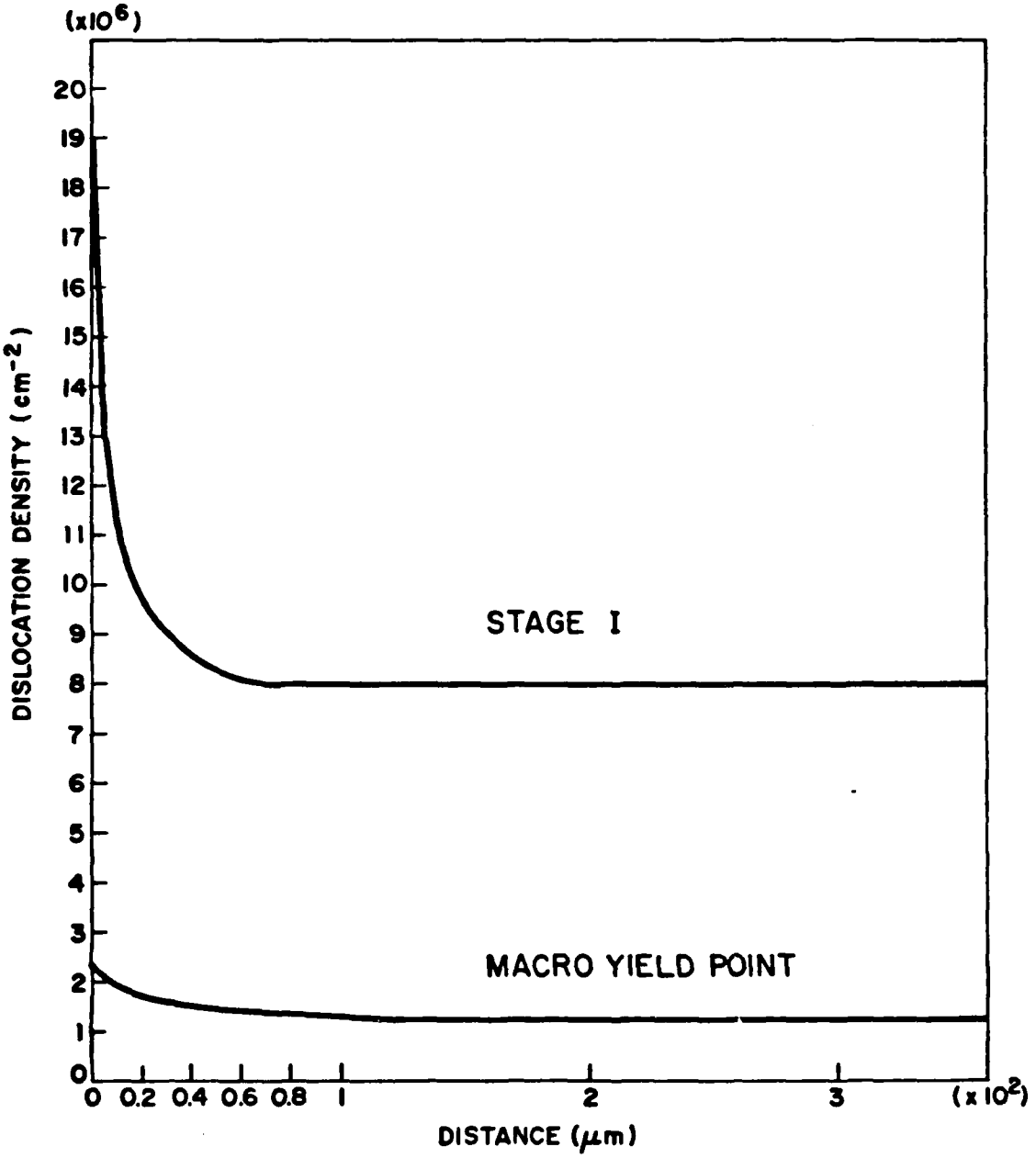


Fig. 1. Kitajima's experimental data of dislocation densities vs. distance beneath the surface, for plastically deformed Cu single crystals at the beginning of macro yield point and during stage I, respectively.

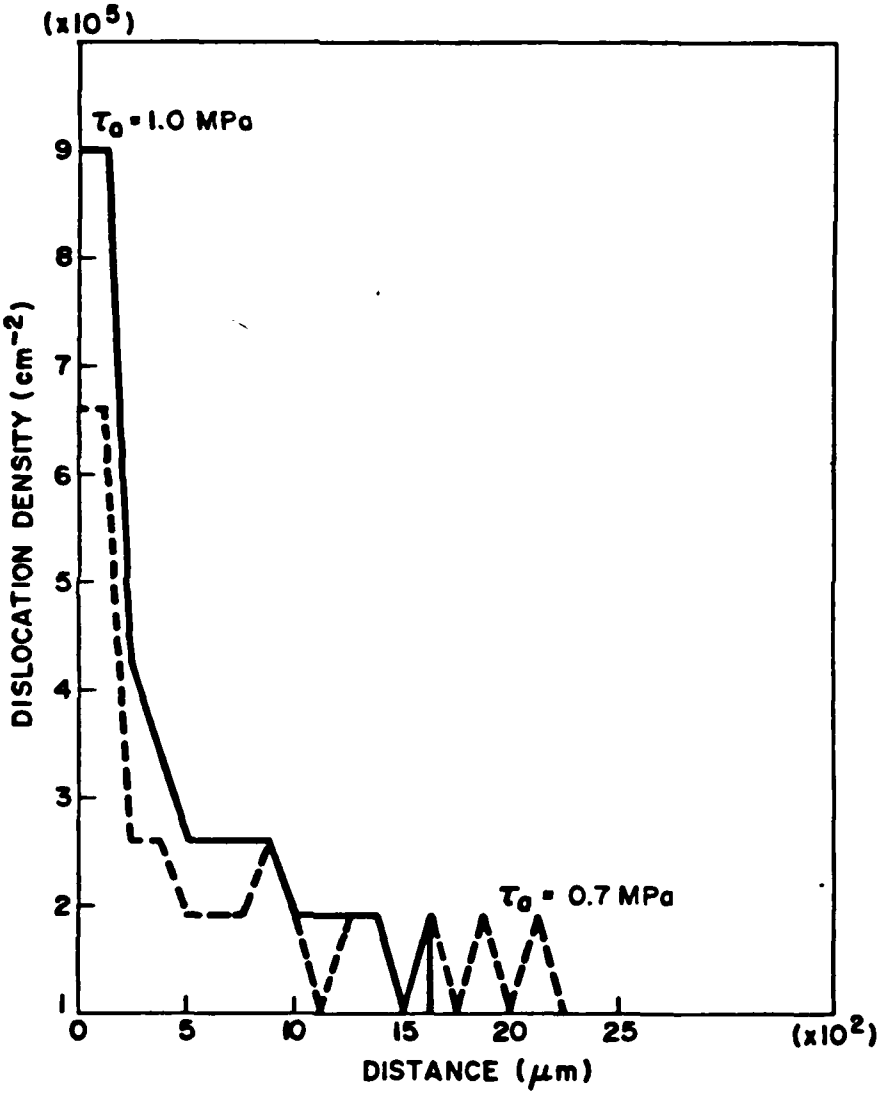


Fig. 2. The effect of different levels of applied stress for the barrier model of Cu, at 298K, with 30 dislocations generated in each case.

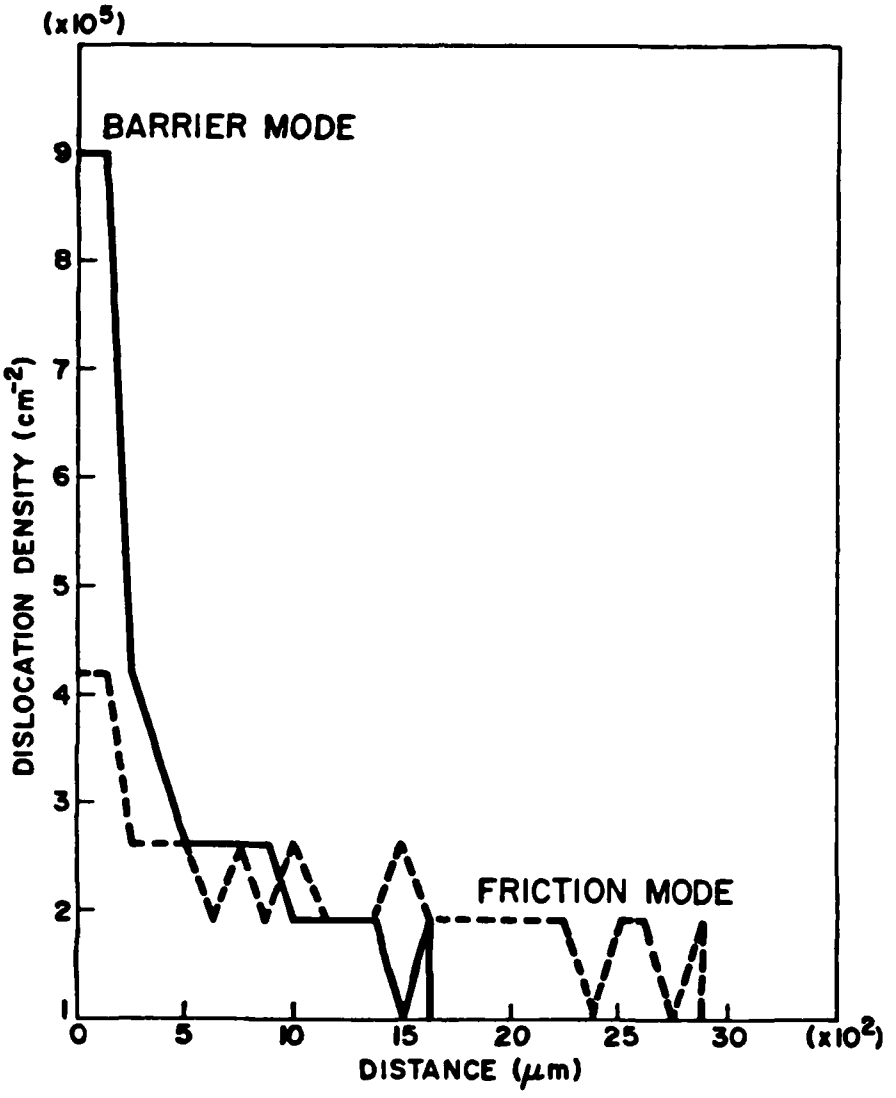


Fig. 3. The comparison between the barrier and the friction models for Cu at constant τ_a = 1 MPa, 298K, with 30 dislocations generated in each case.

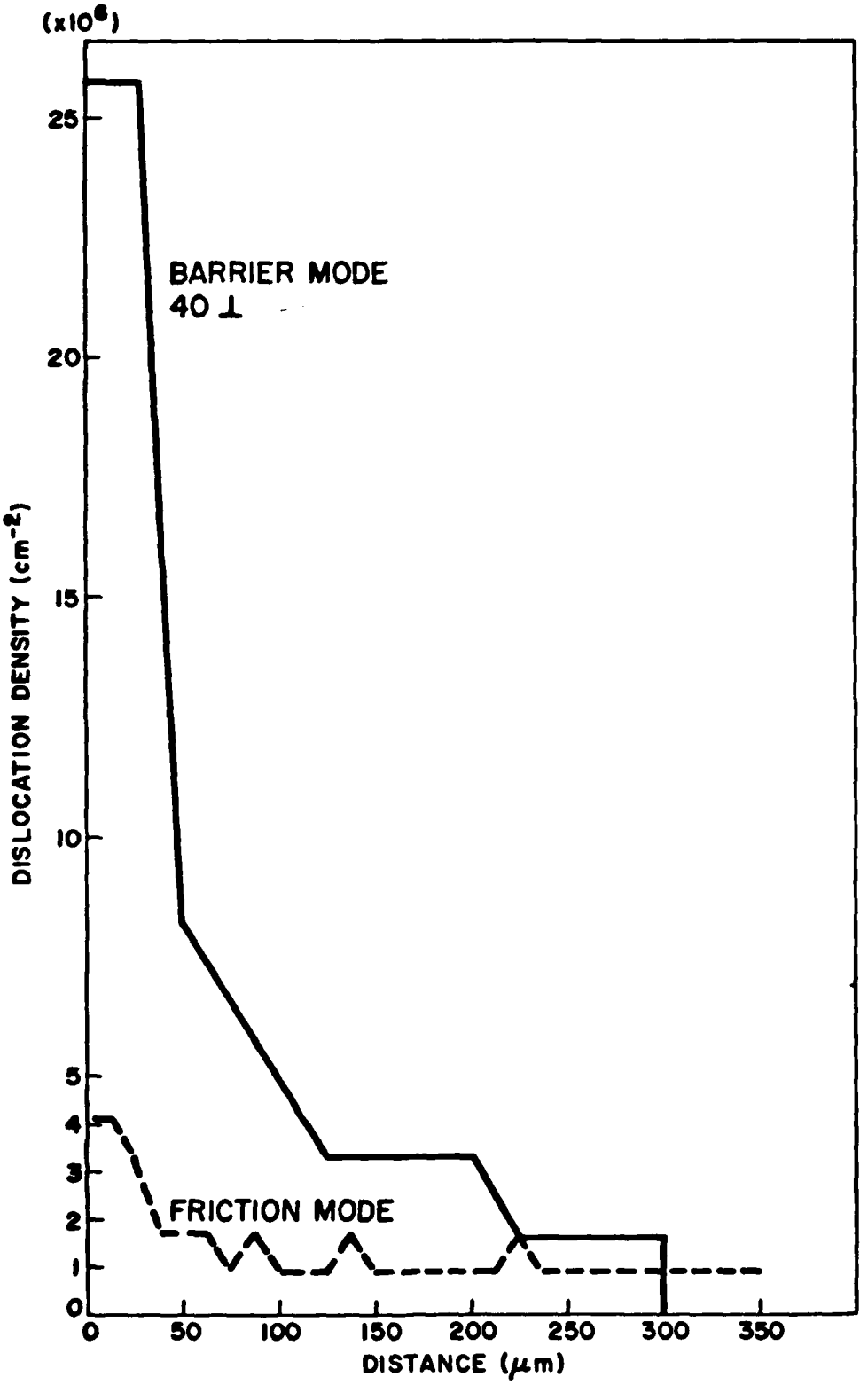
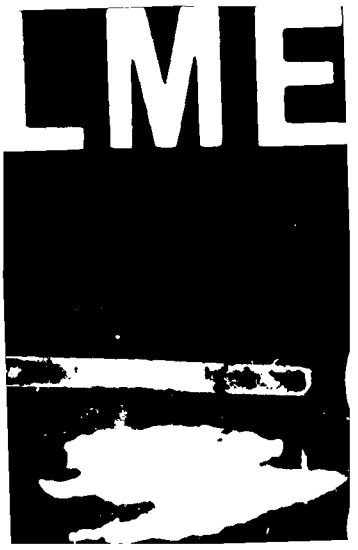


Fig. 4. The comparison between the barrier and the friction models for Fe-Si at constant $\tau_a = 10^2$ MPa, 298K, with 40 dislocations generated in each case.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